Solitonic approach to the dimerization problem in correlated one-dimensional systems

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Using exact diagonalizations we consider self-consistently the lattice distortions in odd Peierls-Hubbard and spin-Peierls periodic rings in the adiabatic harmonic approximation. From the tails of the inherent spin soliton the dimerization d_∞ of regular even rings is found by extrapolations to infinite ring lengths. Considering a wide region of electron-electron onsite interaction values $U > 0$ compared with the band width $4t_0$ at intermediately strong electron-phonon interaction g, known relationships obtained by other methods are reproduced and/or refined within one unified approach: such as the maximum of d_∞ at $U{\simeq}3t_0$ for $g{\simeq}0.5$ and its shift to zero for $g{\to}g_c{\approx}0.7$. The hyperbolic tangent shape of the spin soliton is retained for any U and $g \stackrel{<}{\sim} 0.6$. In the spin-Peierls limit the d_∞ are found to be in agreement with results of DMRG computations.

63.20.Kr, 71.20.Rv, 71.27+a, 71.45.Lr

There is a longstanding debate on the interplay of the electron-electron (*el-el*) interaction and the electron-phonon (*el-ph*) interaction in conducting polymers like *trans*-$(CH)_x$. Among a large amount of papers we refer here only to Refs. 1-6 devoted to the discussion of the origin of the observed dimerization d in the framework of the (extended) Peierls-Hubbard model (PHM). The PHM is regarded as the minimal microscopic model for conducting polymers. Special features of the interplay of on-site correlation U and off-diagonal *el-ph* interaction have been pointed out first in Ref. 1. Employing the Gutzwiller approximation (GA), it was shown that for weak and intermediate *el-ph* interaction strength, the dimerization d passes through a maximum near $U \approx 4t_0$ when U is increased after which it is suddenly suppressed. The geminal approach[6] (GEA) shows a smooth decrease of d with increasing U in the opposite strongly correlated limit. According to extrapolations based on exact diagonalizations (ED)[2,3,5] the enhancement of d due to U predicted by the GA near the maximum is overestimated. In Refs. 2,3 the infinite chain limit d_∞ calculated using the PHM was extrapolated from above (below) by $2n$-membered open chains ($4n$+2- membered rings). In the highly correlated limit of the 1/2-filled band case the PHM can be mapped onto the antiferromagnetic spin-1/2 Heisenberg model (AFHM) and at low temperatures a spin-Peierls phase is expected. Such dimerized phases have been observed for $CuGeO_3$ (having CuO_2 chains) and α'-NaV_2O_5. The CuO_3 chains in $Sr(Ca)_2CuO_3$ are at the threshold to the AFHM-limit[7]. In many cases of practical interest the actual d is very small and no self-consistent $d \neq 0$ is found in feasible short *even* rings.

In the present paper we show that studies of *odd* rings of comparable lengths yield reliable estimates of lattice distortions in infinite rings at arbitrary strength of *el-el* correlations and reasonable strength of the *el-ph* interaction. We exploit the generic property of neutral odd periodic rings that their ground state is given by a spin soliton. The lattice distortions for such a ring are shown schematically in Fig. 1. The bond in front of the soliton center, i.e. between sites N and 1, is a long bond for which a_{N1}-a_0=$2u_0 \equiv d > 0$ holds (a_{N1} (a_0) is the bond-length in the distorted (equidistant) state). For large N the region far from the soliton center tends to the regularly dimerized state. Hence, varying the model parameters, insight into the behavior of d_∞ may be gained already at finite N from the study of d. For short rings ($N = 3, 5, .$), $d(N)$ exceeds significantly d_∞. This is the consequence of a strong first-order Jahn-Teller effect[8]. In Refs. 8,9 the total energy $E_{\rm tot}$ of odd AFHM rings has been studied for *fixed* geometries adopting rigid sharp soliton shapes. In our method *all* bonds are optimized to yield the minimum of the total energy $E_{\rm tot}$. The inherent soliton exhibits a *smooth* shape. We illustrate our method considering the PHM and the AFHM, where comparison with other reliable approaches is possible. In particular, the density matrix renormalization group is used to check the extrapolated d_∞.

For the electronic part $H_{\rm el}$ of the total Hamiltonian $H = H_{\rm el} + H_{\rm lat}$ we adopt the one-band extended PHM

$$H_{\rm el} = \sum_{i,s} t_{i,i+1} \left(c^\dagger_{i,s} c_{i+1,s} + \text{H.c.} \right) + \\ + \sum_i \left(U n_{i,\uparrow} n_{i,\downarrow} + V_{i,i+1} n_i n_{i+1} \right), \tag{1}$$

at half filling, where $c^\dagger_{i,s}$ creates an electron with spin s=$\pm 1/2$ at site i, $n_{i,s}$=$c^\dagger_{is} c_{is}$ is the number operator,

and n_i=$\sum_s n_{is}$. We linearize the bond-length dependent transfer integral t and the intersite *el-el* interaction V

$$t_{i,i+1} = -\left(t_0 - \gamma v_i\right), \quad V_{i,i+1} = V - \eta v_i, \tag{2}$$

where v_i=u_{i+1}-u_i, u_i is the displacement of the $i^{\rm th}$ site relative to the undistorted state. In the adiabatic and harmonic approximation the lattice part $H_{\rm lat}$ reads as

$$H_{\rm lat} = (K/2)\sum_i v_i^2, \tag{3}$$

where K is the spring constant. Via the Hellmann-Feynman theorem we obtain N self-consistent Eqs.

$$Kv_i = \Lambda/N - 2\gamma P_{i,i+1} + \eta D_{i,i+1}, \tag{4}$$

where Λ=$\sum_i \left(2\gamma P_{i,i+1} - \eta D_{i,i+1}\right)$ expresses the fixed length constraint $\sum_i v_i = 0$, $P_{i,i+1}$ being the bond order, and $D_{i,i+1}$ denotes the density-density correlators in the ground state $\mid G\rangle$

$$P_{i,i+1} = \frac{1}{2}\sum_s \langle G \mid c_{i,s}^\dagger c_{i+1,s} + \text{H.c.} \mid G\rangle, \tag{5}$$

$$D_{i,i+1} = \langle G \mid n_i n_{i+1} \mid G\rangle. \tag{6}$$

The strength of the *el-ph* interaction can be measured by the parameter g introduced as[5]

$$g = \gamma/\sqrt{Kt_0} < 1. \tag{7}$$

Note that sometimes[1] the related quantities defined as

$$\lambda_{\rm el-ph} = 2g^2/\pi, \quad \text{or} \quad \lambda_{\rm SSH} = 2\lambda_{\rm el-ph}. \tag{8}$$

are used. Values of $g \sim 0.4$ to 0.5 typical for conducting polymers are regarded as weak to intermediate coupling constants. Following Refs. 5,6 we shall use hereafter the dimensionless dimerization defined as

$$d = 2u_0\sqrt{K/t_0} < 1. \tag{9}$$

The parameter δ frequently used to describe the modulation of the transfer integral $t_{i,i+1} = t_0(1+(-1)^{i+1}\delta)$ in the dimerized state[1-3] is related to d by $\delta = gd$. In the limit $U/t_0 \gg 1$ the low-energy physics of the 1/2-filled PHM ring (Eq. (1)) can be described by the AFHM

$$H_{\rm sp} = \sum_i J_{i,i+1}\vec{S}_i\vec{S}_{i+1}, \text{ with } J_{i,i+1} \approx \frac{4t_{i,i+1}^2}{U - V_{i,i+1}} \tag{10}$$

where the exchange integral is given to 2^{nd} order perturbation theory in t_0/U. Using Eq. (2) we find

$$J_{i,i+1} = J_0 - \gamma_{\rm sp} v_i = J_0(1 + (-1)^{i+1}\delta_{\rm sp}), \tag{11}$$

where $\gamma_{\rm sp}$=$2\gamma J_0/t_0$ and $\delta_{\rm sp}$=$2gd$ characterizes the regular spin-Peierls state for η=0. We shall use the AFHM also out of the limit $U \gg t_0$ for the case V=0 adopting an effective exchange integral J=$J(U/t_0)$ given by the relation J_{ij}=$(2/\pi)v_{\rm sp}t_{ij}$ and the spin velocity $v_{\rm sp}$ taken from the Bethe-Ansatz solution for the equidistant infinite Hubbard ring[10] (hereafter a_0=1, $\hbar$=1)

$$J_{i,i+1} = \frac{4}{\pi}\frac{t_{i,i+1}I_1(z_{i,i+1})}{I_0(z_{i,i+1})}, \quad z_{i,i+1} = \frac{2}{\pi U}t_{i,i+1}, \tag{12}$$

where I_n, $(n = 0, 1)$ are modified Bessel functions.

Using the Lánczos-method, the Hamiltonians (Eqs. (1, 10)) have been diagonalized exactly for finite rings with periodic boundary conditions starting with a given set $\{v_{n,(0)}\}$. The AFHM has been treated using the spinless fermion technique[11] resulting in analogous self-consistent equations as for the PHM. Then the corresponding "ground-state" eigenvector $\mid G\rangle$ has been used to calculate the next set of lattice order parameters $\{v_{n,(1)}\}$ using Eq. (4). The iteration was continued until the maximal deviations of $E_{\rm tot}$ and all $v_{n,(j)}$ between two iteration steps j and $j+1$ became smaller than the required accuracy of 10^{-7} to 10^{-8} (see Refs. 3,12). Here rings composed of up to N=13 sites (PHM) and N=23 (AFHM) have been studied. The ED computer limitations to rings where finite size effects are still important can be circumvented at least for *even* membered regularly dimerized AFHM rings and reasonable *el-ph* (*sp-ph*) interaction strength applying the density matrix renormalization group technique[13] (DMRG) with typical discarded errors of the order 10^{-6}.

At first we consider the one-particle Su-Schrieffer-Heeger model (SSH) (PHM: U,V=0) where very long odd rings can be treated numerically. The infinite even ring problem is reduced to a transcendental equation for d_∞:

$$\frac{1}{\lambda_{\rm SSH}} = \frac{K(k) - E(k)}{k^2}, \quad \text{with} \quad k = \sqrt{1-(gd_\infty)^2}, \tag{13}$$

where K and E denote complete elliptical integrals. The results for up to $N = 601$ sites are shown in Fig. 2. Starting from small N, d passes at first by a minimum at $N \simeq 2\xi$, the width of a soliton in an infinite ring. For weak *el-ph* coupling $\xi \gg 1$, $d_{\rm min}/d_\infty \approx 0.86$ at $2\xi/N \approx 0.92$. Below that minimum all curves, for which $N > 2\xi$ holds, approach a nearly universal curve, pass a very small maximum near 6ξ, and tend finally to d_∞ from above[14]. Since for correlated problems only relatively short rings can be treated exactly, a strong nonmonotonous behavior could cause problems in extrapolating to d_∞. Fortunately, our calculations indicate that at least in the AFHM-limit the depth of the first minimum at finite N is strongly suppressed.

Let us now consider how the on-site interaction U affects d. As shown in Fig. 3 starting from $U = 0$, d increases with U and has a maximum at $U_{\rm max} \sim 3t_0$, after which d starts to decrease smoothly. Both behaviors are similar to the GA and GEA predictions, respectively. Quantitatively, however, we obtain $U_{\rm max}(g)$≈$3.12t_0$ for

$g \sim 0.5$. For $0.5 < g < 0.6$, $U_{\max}$ starts to decrease. Finally, when $g \to g_c \approx 0.7$, $U_{\max} \to 0$. For comparison we note that the GA's results are $U_{\max} \approx 4t_0$ for $g < g_c = 0.76$. The ED-results of Ref. 5 yield $g_c = 0.75 \pm 0.04$ slightly above our result. Above g_c, there is no enhancement of d due to U. Turning to larger rings, we first adopt an $1/N$ extrapolation (dashed curve) and arrive at a rough lower bound being crudest for small U. An improved bound is achieved connecting the exact $U=0$ point with the $1/N$ extrapolation upshifted to the AFHM limit (see below). To avoid an artificial minimum, we omit the $U=t_0$ point. Thus for $g=0.5$ we get $0.174 < d_{\infty,\max} \lesssim d_{N=13} \approx 0.2$. Instead the GA[6] gives $d_{\max} \approx 0.31$. For $U \gg t_0$, $g \leq 0.5$ the $d_{\rm PHM} \to d_{\rm AFHM}$ from above. To compare our d with the continuum model result of Inagaki et *al.*[16], we rewrite their dimerization as

$$d = \frac{g^2}{\pi\sqrt{1+\kappa}} \left(\frac{\partial J_0}{\partial t_0}\right)^2 \left(\frac{t_0}{J_0}\right)^{1/2} \to c g^2 \left(\frac{4t_0}{U-V}\right)^{3/2}, \tag{14}$$

where $c = (4/\pi)\sqrt{2/3} \approx 1.04$ for $\kappa = 0.5$ (see Eq. (10) and Refs. 16 -18). Applying Eq. (14) to intermediately correlated cases, we adopt the effective exchange integral J defined by Eq. (12) and arrive at an *analytic* expression (the dashed-dotted curve in Fig. 3)[18]. Surprisingly it exhibits similar shape and magnitude as the weak coupling ($g \leq 0.5$) ED-curves. In particular its $U_{\max}/t_0 = 3.21$ is close to 3.12 mentioned above. This suggests that even in the case of conducting polymers, being clearly outside the usual AFHM-regime, the dimerization is mainly governed by the (always present) spin degrees of freedom and to less extent by the charge degrees of freedom. In the usual case $U > 2V$, the V and its derivative η (see Eq. (2)) enhance d. For $U \gg t_0, V$ and $\eta = 0$ one can replace $U \to U - V$.

For long rings $N > 2\xi$, d_N-values close to d_∞ can be expected. Then $d = d(N)$ might be approximated by

$$d(N) = d_\infty + \sum_{l=1}^{l_{max}} \frac{A_l}{N^l} \exp\left(\frac{-N}{2\xi}\right) \quad + ... \quad . \tag{15}$$

Note that in contrast with the general PHM case, $d(N)$ for $4n$ and $4n+2$ AFHM-rings can be described by *one* smooth curve[8]. The $d_{\rm even} \to d_\infty$ from below, just opposite to odd rings. To be specific, we consider one typical example. We estimate for the upper curve shown in Fig. 4, $d_{\rm odd,\infty} = 0.0765$, $l_{max} = 1$, $A_{1,\rm odd} \approx 0.5$ and $\xi_{\rm odd} = 5.26$. The even ring curve tends from below to a slightly larger value $d_{\rm even,\infty} = 0.078$ and $A_{1,\rm even} = -11.8$. The exponent $\xi_{\rm even} = 1.85$ differs significantly from $\xi_{\rm odd}$. From the soliton shape $(-1)^n v_n \approx d_N \tanh(n/\xi_N)$, we deduced at $N=23$, $\xi_N \approx 5$, $d_N \approx 0.08$, whereas the continuum model[17] yields $\xi = 3\pi t_0/(16 J_0 g^2) = 4.91$. The fit of the even curve can be somewhat improved adopting $l_{max} = 4$. Then with $A_1 = A_3 = 0$ and $A_2 = -3.5, A_4 = -2040$ one arrives at the same $\xi = 5.26$ as in the odd case for $l_{max} = 1$. Taking the DMRG-values for $N=60$, we conclude that the accuracy of the solitonic estimate of d_∞ is ~ 2 to 3 %. The continuum theory[16], (Eq. (14)) predicts, for $\kappa = 0.5$, $d_\infty = 0.07203$, a value slightly below our discrete results. According to our numerical finding we would recommend to use $\kappa \approx 0.279$. Fitting alternatively the curvature of $d_{\rm odd}$ at large N by a parabola, one arrives at an extrapolated very shallow minimum at *finite* ring length ($N_{\min} \approx 29$ sites for the present parameters). Then the slightly smaller $d_{\infty,\rm odd}$ compared with $d_{\infty,\rm even}$ might be viewed as a hint for a tiny minimum at *finite* N generic for d_{odd} being the deepest in the SHH case (see Fig. 2). Raising g, the soliton becomes narrower. Thus at large g any minimum should be accessible by the ED. With increasing g the $d_{\rm odd}(1/N)$ curves become flatter. Small minima were detected for $g=0.9$, 0.85 at $N = N_{\min} = 17$, 21, respectively. Anyhow, the $1/N$-extrapolation of $d_{\rm odd}$ ($d_{\rm even}$) from accessible $N \leq N_{\min}$ yields a lower (upper) bound of d_∞.

To summarize, a novel approach to the dimerization problem of correlated 1D-models has been presented. It is based on exact diagonalizations of odd ring Hamiltonians combined with a self-consistent treatment of the classical lattice degrees of freedom. Known dependences of the bond alternation on the *el-el* and *el-ph* coupling strengths obtained by other approximations valid in different parameter regimes have been reproduced and refined within one unified method. The $1/N$-extrapolation to the infinite rings gives a new lower bound for any correlation strength. With the aid of the Bethe-Ansatz solution for the spin velocity, even in the intermediate coupling regime a sizeable part of the dimerization can be described by an effective spin-Hamiltonian gaining thus new insights in the dimerization mechanism of conducting polymers. The DMRG is found out as a valuable supplementary tool to our solitonic method.

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FIG. 1 Schematical view of the lattice distortions in 1/2-filled odd rings. (Un)distorted sites are denoted by $\circ(\bullet)$.

FIG. 2 Reduced dimerization in odd SSH rings *vs*. reciprocal ring length $1/N$ for various *el-ph* interactions g. The ring length N is given in units of the soliton width $2\xi=2/(gd_\infty)$.

FIG. 3 Dimerization in the Peierls-Hubbard model *vs.* on-site energy U for the *el-ph* coupling g=0.5. In deriving the improved lower bound, Eqs. (13-15) have been used.

FIG. 4 Size dependence of the dimerization d for even ($\circ$) and odd ($\bullet$) periodic spin-Peierls rings. Even rings are treated by ED until N=22. The d for N=28 to 60 are obtained by the DMRG. The parameter set used $\gamma_{\rm sp}$=0.4, J=1/3, K=1 corresponds to U=13,V=t_0=1,η=0, and g=0.6 for the PHM. The full and the dashed curves are the fits by Eq. (15).

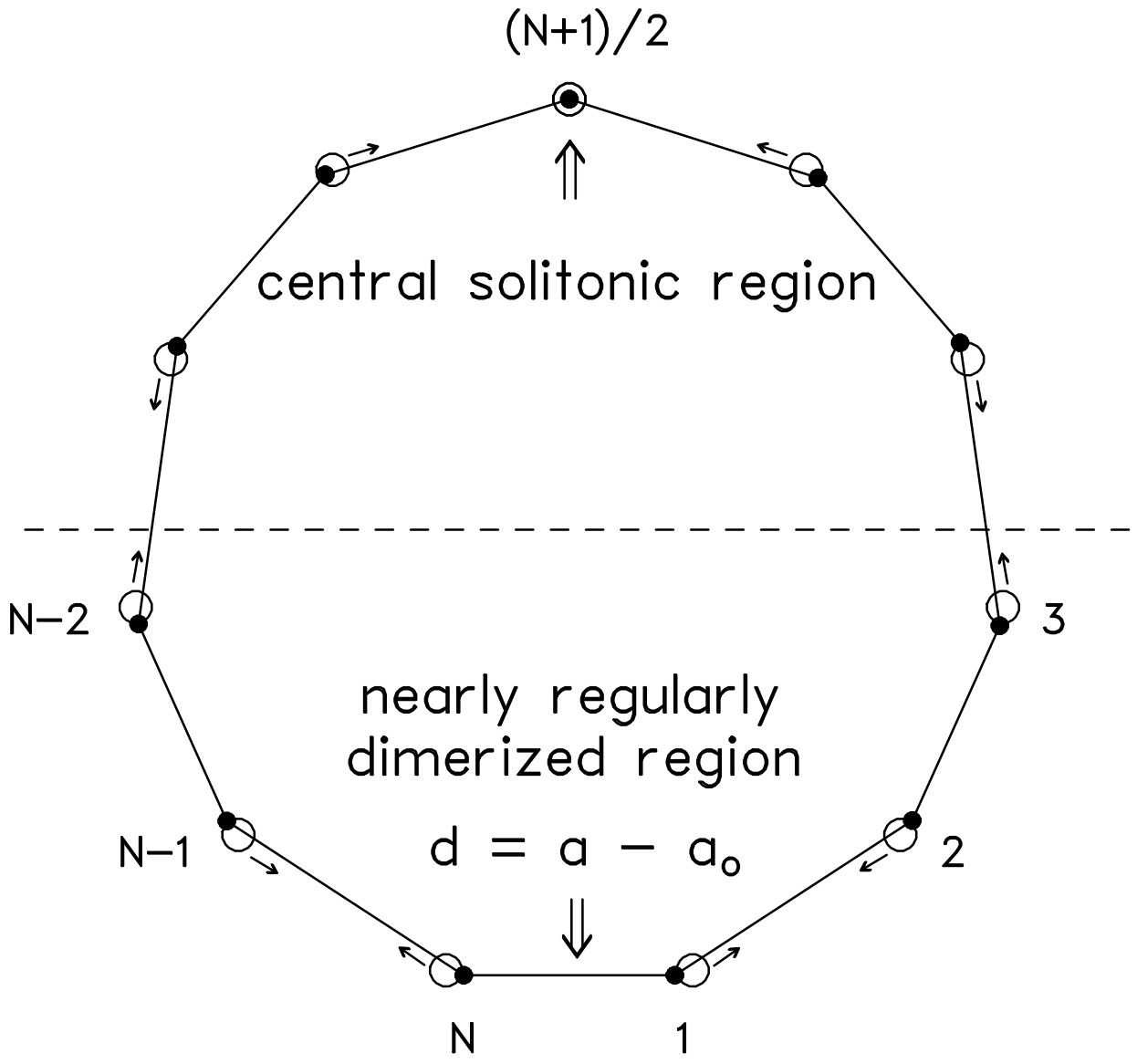

Fig. 1

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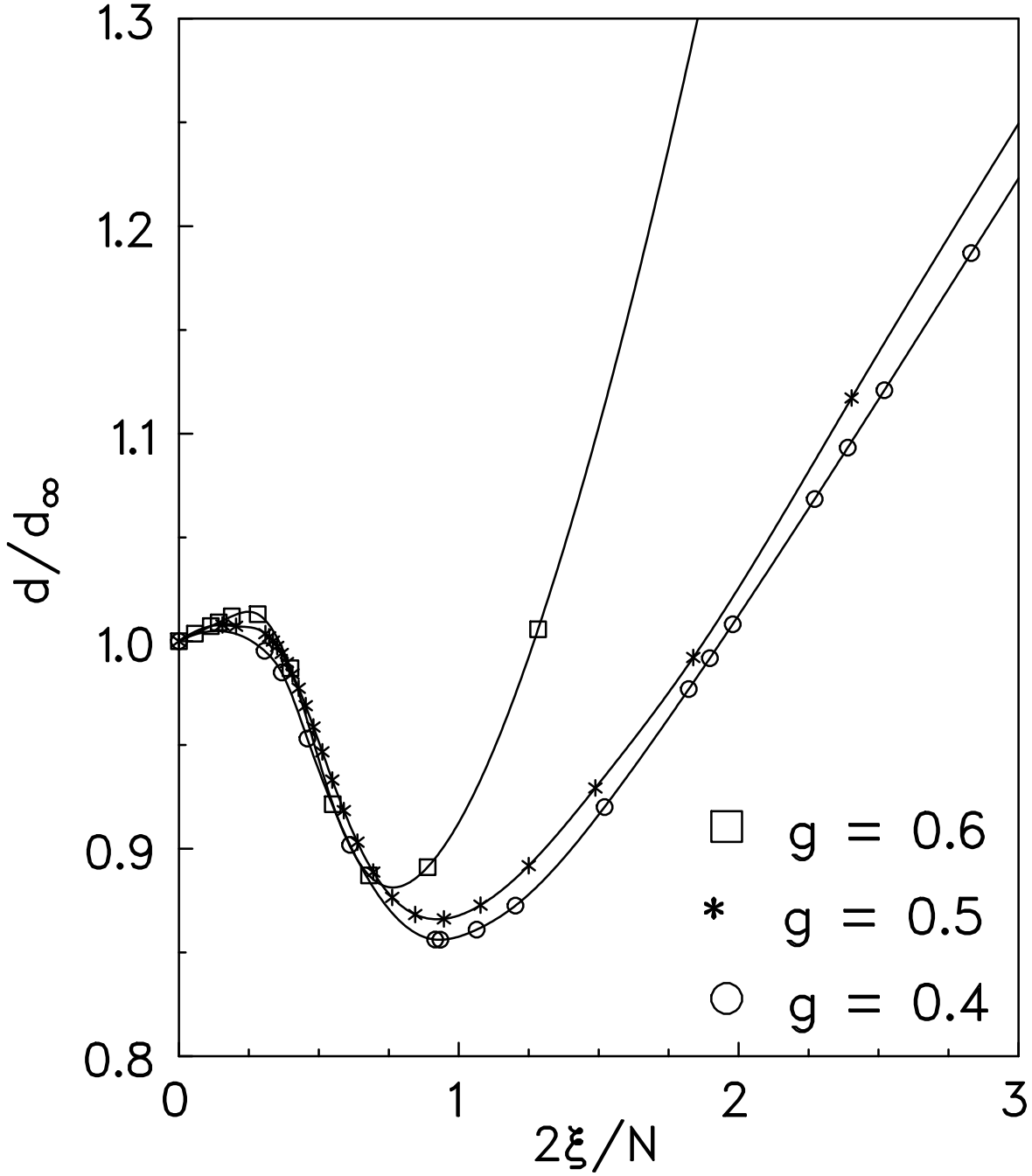

FIG. 2 Malek et al.

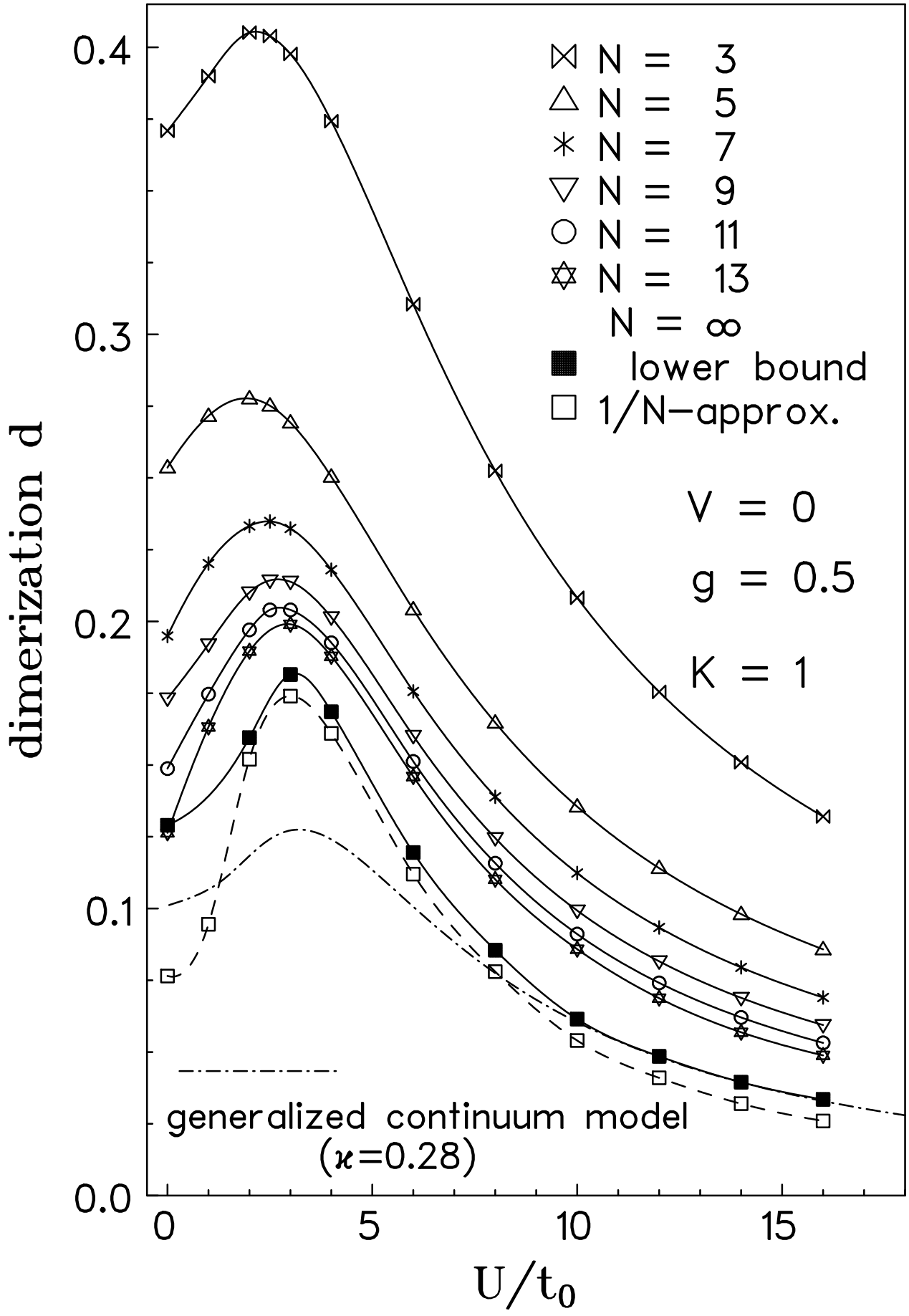

Fig. 3 Malek et al.

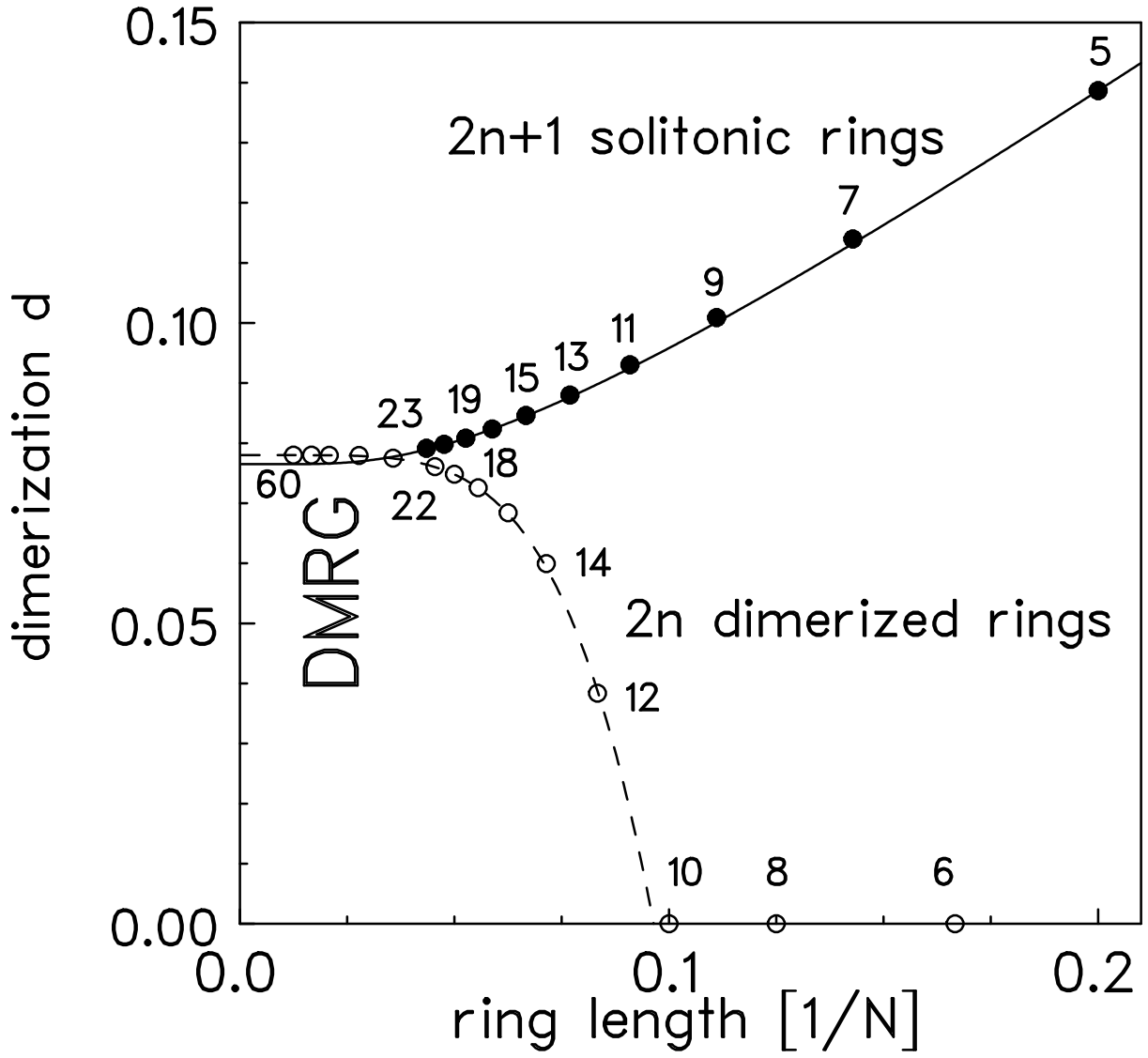

Fig. 4

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